Infinite set of crossover exponents of the XY model and $f(\alpha)$ approach

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For transitions described by the XY model, it has been shown that each Fourier component of the angular-structure factor is controlled by a different crossover exponent. Each crossover exponent is associated with a particular symmetry-breaking field. It is shown here that although, as for multifractals, the angular structure itself can be obtained from the crossover exponents, in contrast to multifractals, the asymptotic form of this angular-structure factor is described by the Legendre transform of the (analytically continued) infinite set of crossover exponents only in the special case of two dimensions.

I. INTRODUCTION

Infinite sets of crossover exponents were calculated early after the introduction of the renormalization group in critical phenomena.[1,2] Attention was usually focused on a few relevant exponents, even though a given universality class is in fact characterized by all its exponents, including, in particular, all possible crossover exponents. This focus on a few exponents is justified since observable quantities in general couple to many renormalization-group eigenoperators and hence are controlled only by the most relevant ones.

In certain cases, a very large (in principle, infinite) number of crossover exponents is, nevertheless, experimentally measurable. This was achieved probably for the first time in 1974 in neutron-diffraction experiments on the magnetic structure factor of erbium.[3] It is, however, only with the work of Cowley and Bruce[4] in 1978, Per Bak[5] in 1980 and Brock[6] *et al.*[6] in 1986 that the true significance of that work became clear. In all the different physical cases treated by these authors, one is accessing experimentally part of the infinite set of crossover exponents associated with each possible symmetry-breaking operator for the three- or two-dimensional[7] XY model. In the limit where phase fluctuations are important, higher-order harmonics of the basic frequency ("secondary-order parameters" of Cowley and Bruce[4]) indeed couple to different renormalization-group eigendirections.

In the context of electrical properties of percolating clusters,[8] diffusion-limited aggregates,[9] and localization,[10] the appearance of infinite sets of exponents[11] has become known under the name "multifractal" after corresponding works in turbulence[12] and dynamical systems.[13] In the latter case, a detailed geometrical interpretation was given to the Legendre transform of the infinite set of exponents seen as a continuous function.[13] This has become known as the $f(\alpha)$ function. In the first three cases mentioned above, the $f(\alpha)$ function simply characterizes the scaling properties of a probability distribution in the limit where the logarithm of the scaling length (system size or correlation length) becomes large. In the present paper, we wish to show that the analogous analysis in the case of the XY model in critical phenomena does not lead to a $f(\alpha)$ function except, after analytic continuation, in the special case of two dimensions.

II. INFINITE SET OF OBSERVABLE EXPONENTS FOR THE XY MODEL

We first recall how an infinite set of measurable exponents appears for the XY model. The following analysis should apply[4,5] to phase transitions characterized by a complex order parameter in general,[4] such as commensurate-incommensurate transitions, and melting transitions[5] in graphite intercalates. To be specific we remind the reader of the case studied by Aharony *et al.*[6] Consider the S_A-S_{BH} or S_C-S_I liquid-crystal transitions. (The two smectic liquid crystal phases, S_{BH} and S_I, also have hexatic symmetry.) The starting Ginzburg-Landau Hamiltonian[14] is

$$H=\int d^dr[\tfrac{1}{2}|\nabla\Psi|^2+\tfrac{1}{2}r|\Psi|^2+u_4|\Psi|^4+u_6|\Psi|^6 +h\,\mathrm{Re}(\Psi)]\ , \qquad (1)$$

where h vanishes in the S_A phase and is small in the S_C phase, while

$$\Psi=e^{6i\vartheta(r)} \qquad (2)$$

is the local order parameter describing the sixfold symmetric orientational alignment of the lines connecting neighboring molecules in the smectic liquid-crystal planes. u_4 is supposed larger than the value where the model is tricritical. The Hamiltonian (1) then describes the XY model. Through measurements of higher-order Fourier components of the x-ray spectrum[6] in the S_C phase, where the small h introduces long-range hexatic order, the following quantities become experimentally accessible:

$$C_{6n}\equiv\mathrm{Re}\langle\int d^dr\,\Psi^n(r)\rangle\ . \qquad (3)$$

To determine the scaling behavior of these quantities, a symmetry-breaking term[6]

$$H_n \equiv g_n \int d^d r \, \mathrm{Re}(\Psi^n) \tag{4}$$

is added to the Hamiltonian (1). Asymptotically close to the XY fixed point, the free energy should scale as

$$F(t,g_n)=|t|^{2-\alpha} f(g_n/|t|^{\phi_n}) ,$$

where $T=(T-T_c)/T_c$, α is the XY specific-heat exponent, and ϕ_n the appropriate crossover exponent. Thus,

$$C_{6n} = \partial F/\partial g_n|_{g_n=0} \sim |t|^{2-\alpha-\phi_n} . \tag{5}$$

Using the hyperscaling relation $(2-\alpha)=d\nu$ and $|t| \sim \xi^{-1/\nu}$, where ξ is the correlation length and ν the corresponding exponent, we can rewrite (5) as

$$C_{6n} \sim \xi^{-d} \xi^{\phi_n/\nu} . \tag{6}$$

When hyperscaling is valid, one can interpret $(L/\xi)^d$ as the number of coherence volumes within the system of linear size L in d dimensions. Hence, for $L \ll \xi$,

$$C_{6n} \sim L^{\phi_n/\nu} . \tag{7}$$

The crossover exponents ϕ_n are not[6] a linear function of n, except in mean-field theory. In the present case, the perturbations $|g_n|>0$ are relevant ($\phi_n>0$) for $n \le 3$, and irrelevant otherwise.

III. ASYMPTOTIC FORM OF THE ANGULAR STRUCTURE FACTOR

Multifractals in the context of percolation, localization, and diffusion-limited aggregation first appeared as an infinite set of measurable quantities, each scaling with an exponent which is not a linear function of some basic (gap) exponent. It is only later that it was realized that the measurable quantities are moments of a probability distribution whose asymptotic form, (limit $\ln\xi \to \infty$), as found by a saddle-point integration,[13,15] is simply extracted from the infinite set of exponents by Legendre transformation [$f(\alpha)$ function]. In the present context of the XY model, it is the angular structure factor—the equivalent of the probability distribution for multifractals—which is measured experimentally, while the scaling quantities, the C_{6n}, are extracted by Brock[6] *et al.* from the Fourier analysis of the angular dependence of this scattered intensity $S(\chi)$ [$S(\chi)$ is a positive, even function of χ which can also be interpreted as a probability]:

$$S(\chi) = I_0 \left[\tfrac{1}{2} + \sum_{n=1}^{\infty} C_{6n} \cos[6n(\chi - 90^\circ)] \right] + I_{\mathrm{BG}} . \tag{8}$$

The question of the asymptotic form of $S(\chi)$ (limit $\ln\xi \to \infty$) then arises. To find out whether it is related to the Legendre transform of the exponents for C_{6n}, we proceed as follows. Defining $\theta=6(\chi-90^\circ)$ and $S_1(\theta) = S(\chi)$, and dropping the background contribution I_{BG}, we are left with

$$S_1(\theta) = \sum_{n=-\infty}^{\infty} M(n) e^{in\theta} , \tag{9}$$

where the Fourier coefficients are given by

$$M(n) = \frac{I_0 C_{6n}}{2} = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} S_1(\theta) e^{in\theta} . \tag{10}$$

Using the Poisson summation formula, Eq. (9) may be rewritten as

$$S_1(\theta) = \sum_{m=-\infty}^{\infty} \tilde{S}(\theta - 2\pi m) , \tag{11}$$

with

$$\tilde{S}(\theta) = \int_{-\infty}^{\infty} d\omega \, e^{i\omega\theta} M(\omega) , \tag{12}$$

where $M(\omega)$ is defined by Eq. (10) with n taking real instead of integer values. From Eq. (6) we know that in the asymptotic limit,

$$M(n) \approx A(n) \xi^{-d} \xi^{\phi_n/\nu} . \tag{13}$$

Comparing Eqs. (13), (6), and (7) with the corresponding case in percolation, we define

$$\tau(n) \equiv -\phi_n/\nu . \tag{14}$$

Note that by their definitions (10), (13), and (14), ϕ_n or $\tau(n)$ are even functions of n so that Eq. (12) is now rewritten as

$$\tilde{S}(\theta) = 2\,\mathrm{Re} \int_0^{+\infty} d\omega \exp\left[\ln\xi \left[i\omega \frac{\theta}{\ln\xi} + \frac{\ln A(\omega)}{\ln\xi} - d - \tau(\omega) \right] \right] . \tag{15}$$

Note that the use of the Poisson summation formula has allowed us to continue the discrete set of exponents to a continuous one.[16] A continuation from a discrete set to a continuous one is also possible in the usual case of multifractals.[17,18]

We are now in a position to study the asymptotic form of (15). We assume that the amplitudes $A(\omega)$ depend weakly on ω so that these are assumed to lead to an overall constant in the asymptotic evaluation of (15). In fact, the experiment of Brock *et al.*[6] was analyzed by assuming that these amplitudes were completely independent of ω. In the standard cases of multifractals, one can evaluate the analog[19] of Eq. (15) by using general monotonicity and convexity properties to do a saddle-point integration. This leads one to characterize the probability distribution [analog of $\tilde{S}(\theta)$] by the Legendre transform of $\tau(\omega)$. In the present case, since the $\tau(\omega)$ are related to Fourier coefficients instead of moments of a probability, one cannot prove such general convexity properties outside a specific theory for the XY model. The asymptotic analysis of (15) instead depends on the explicit form of $\tau(\omega)$ for the XY model. Following the definitions of Aharony *et al.*,[6]

$$d - \frac{\phi_n}{\nu} = \frac{(d-2+\eta)}{2} n + \tfrac{1}{2} x_n n(n-1) . \tag{16}$$

The ϵ expansion[20] then gives

$$x_n \sim \tfrac{1}{5}\epsilon[1+\tfrac{1}{5}\epsilon(3-n)+\tfrac{1}{25}\epsilon^2(n^2+3.666\,455n-22.322\,657)] , \qquad (17)$$

while, using the numerical values of the diagrammatic integrals evaluated by Jug[21] in three dimensions, Aharony *et al.*[6] obtain

$$x_n \sim \frac{0.3}{1+0.027n} . \qquad (18)$$

Paczuski and Kardar[22] have also proposed the following interpolation formula in the interval $2 \le d \le 4$:

$$x_n = (d-2+\eta)(\epsilon/10+\epsilon^2/5) . \qquad (19)$$

All odd powers of n in the results (16) to (19) must be interpreted as absolute values, i.e., $\tau(n)$ is an even function of n. Despite the differences between these results, especially at large values of n, where they are less reliable, they all correspond to functions $\tau(\omega)$ which are monotone decreasing functions of ω for $\omega \ge 0$. We assume then that the above property is a general consequence of the renormalization-group description of the critical properties of the XY model. Returning to (15), the saddle point nearest to the contour of integration in all these cases is at negative values of $\mathrm{Re}(\omega)$, i.e., outside the contour of integration. Deforming the contour of integration to go along the stationary phase path is not particularly useful in the present case.[23] The asymptotic form of $\tilde{S}(\theta)$ then, is not given by the $f(\alpha)$ form commonly encountered in multifractals. Instead, one obtains,[23] in the limit $\theta/\ln\xi$ finite, $\ln\xi \to \infty$,

$$\tilde{S}(\theta) = 2\,\mathrm{Re}\left[\frac{1}{\ln\xi}\frac{1}{i\alpha+\tau'(0)} - \frac{1}{(\ln\xi)^2}\frac{\tau''(0)}{[i\alpha+\tau'(0)]^3} + \cdots\right] , \qquad (20)$$

where τ' and τ'' denote, respectively, the first and second derivative of τ and

$$\alpha \equiv \frac{-\theta}{\ln\xi} . \qquad (21)$$

Note that although α appears as a natural variable for that expansion of $\tilde{S}(\theta)$, (11) implies that this is not true for the observed quantity (8).

Equation (15) could not be evaluated in the saddle-point approximation because of the particular functional form of the $\tau(n)$, not because the $\tau(n)$ are discrete. The functional form $\tau(n)=n^2+an$, for example, which is forbidden by symmetry when n is not interpreted as $|n|$, would have lent itself to saddle-point evaluation.

For the two-dimensional case,[22,7] $d-\phi_n/\nu = n^2/(d-\phi_1/\nu)$ so that $\tau'(0)=0$, invalidating the expansion (20). In that case, the saddle-point evaluation of the integral is indeed exact. There is one and only one saddle point along the pure imaginary axis at $\omega = i\rho$ with ρ real. The convexity of the ϕ_n/ν is then opposite to that of its analytically continued form $-\tau(i\rho)$. In that case, we can write

$$\tilde{S}(\theta) = C(\theta,\ln\xi)\xi^{f(\alpha)-d} , \qquad (22)$$

where $C(\theta,\ln\xi)$ depends weakly on its arguments and where $f(\alpha)$ is the Legendre transform of the real function of ρ, $-\tau(i\rho)$, in other words,

$$f(\alpha) \equiv \alpha\rho - \tau(i\rho) , \qquad (23)$$

where as usual, the value of ρ is given by

$$\alpha \equiv \frac{\partial \tau(i\rho)}{\partial \rho} . \qquad (24)$$

$f(\alpha)$ is concave because it is the Legendre transform of a convex function. At its maximum, $f(\alpha)$ is equal to d (usually, it is equal to the fractal dimension of the object under consideration[13]). Note that $f(\alpha)$ may be negative as in the previously mentioned fields[24] and in contrast to the dynamical systems case. Also, $f(\alpha)$ is even and maximum at $\alpha=0$. However, $f(\alpha)$ is here a simple parabola, and (22) is a Gaussian. This is thus a somewhat trivial case which does not justify developing a $f(\alpha)$ formalism. However, if additional corrections to the n dependence beyond the Villain approximation are found later, then the above approach may prove useful.

In closing this section, note that when the field h in Eq. (1) strictly vanishes, the same arguments as above may be repeated but this time for the conditional probability that if θ vanishes at some point, it has a value $\theta(r)$ at distance r. This follows from the fact that

$$\langle \{\mathrm{Re}[\Psi^n(r)]\}\{\mathrm{Re}[\Psi^n(0)]\}\rangle \sim r^{2\phi_n/\nu-2d} \quad (r \ll \xi) . \qquad (25)$$

IV. DISCUSSION AND CONCLUSION

It is now known that a large number of the exponents—in principle all—belonging to the infinite set of exponents associated with symmetry-breaking operators of the group $O(2)$ are accessible experimentally.[6] These exponents characterize the fully symmetric fixed point[1,2] and their observability is clearly associated with their symmetry-breaking aspect rather than with their relevance. In fact, they are irrelevant in the present case for $n \ge 4$. While the probability distribution for angular dependence of the scattered intensity (angular structure factor) can be obtained from the crossover exponents, the asymptotic expansion of that probability distribution is not simply related to the Legendre transform of the crossover exponents, in contrast to the usual case in multifractals. This is not a consequence of the fact that the crossover exponents are discrete. Indeed, for the two-dimensional XY model the Legendre transform *is* simply related to the asymptotic expansion of the probability distribution. Unfortunately this case is a somewhat trivial one. Furthermore, the Legendre transform of the crossover exponents in this case does not seem to have a natural interpretation as a fractal dimension.

We would like to emphasize also that, as in percolation and similar multifractal problems, we expect the angular distribution (or the conditional probability distribution) to converge towards its asymptotic form much more slowly than the moments converge to their scaling form. Indeed, the large parameter of the asymptotic expansion of the probability distribution is only the logarithm of the length scale, which is small in practice. In other words, the renormalization group tells us that the moments scale when the length scale is large while the asymptotic form, and in particular the $f(\alpha)$ form in the case of multifractals, holds when the logarithm of the scale is large.

The problem of the polymer winding number studied by Duplantier and Saleur[25] can be analyzed for the probability distribution as the two-dimensional XY model. In the case of models with $O(n)$ symmetry with $n>2$, more than one angular variable is necessary to describe the eigenfunctions of the irreducible representations.[26] The exponents must then be identified by $n-1$ indices. Although not impossible in principle, it is probably then experimentally not practical when $n>2$ to devise experimental probes for the infinite set of symmetry-breaking operators. This would however be possible in Monte Carlo calculations.

In closing we note that multifractals in percolating systems and in localization are also apparently associated with operators breaking a continuous symmetry but this time in replica space.[26,27,17] Once again, this set is basically discrete but can be continued to a continuous one.[17,18] As in critical phenomena, higher-order susceptibilities of a given observable also obey gap scaling.[17] The observability of the exponents is associated more with symmetry than with relevance. Indeed, in these "standard" multifractal cases, the exponents appear in a "second renormalization group" that contains an additional arbitrary scale factor[26,27] which does not change the original fixed-point properties. Observable exponents in this second renormalization group are "dominant."[27] This difference with standard critical phenomena is the object of other papers.[28]

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